Stress phase space for static granular matter

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Abstract

Some statistical mechanics approaches to jammed granular media are based on ensembles in which the stress state of the system is externally set. This paper proposes a new phase space to describe the microstates of a granular packing compatible to a given macrostate. The nature of this phase space is analyzed, showing that the consideration of the allowed and forbidden regions of every configuration (i.e. geometrical pattern) could be a relevant factor for the establishment of its probability and, therefore, of the expected properties of the sample.
Many combinations of forces acting on a particle can keep it in static equilibrium. Every set of forces could be considered equivalent to a microscopic stress field, but the kind of interaction and the geometrical restrictions mean that not all stress states can be represented by any set. Consequently every local configuration has its respective allowed and forbidden regions in the phase space. As a result, some points of the phase space are degenerate, and the density of states strongly determines the expected statistical distribution in the thermodynamic equilibrium. It is shown how this function just depends on the deviatoric stress. A first analysis of two-dimensional (2D) arrangements is included to clarify this assertion.

1 Introduction

Edwards was the first to propose that a statistical mechanics approach might be feasible to describe dense granular media [1]. Assuming that granular systems have entropy, it was claimed that the volume plays the role of energy (V-ensemble) [1, 2, 3, 4, 5]. There are other formalisms based on the energy of the whole system, such as [6, 7, 8]. Following this work, an approach based on considering the elastic potential energy of particles has recently been presented, referred to as the elastic energy approach [9]. This approach considers the stress state of the system.

In this respect, in recent years, some researchers have suggested that the stress of the system should be considered together with the volume (V–F en-

semble) [10, 11, 12, 13] or even alone (F-ensemble) [14, 15, 16, 12, 17, 18]. This can be done via the force-moment tensor, and this approach is referred to here as the force-moment approach. It uses the concept of angoricity.

Both the elastic energy approach and the force-moment approach consider the external stress as a control parameter. In practice, the main difference between them is whether the statistical weight of the points in the phase space decays as a linear or a quadratic function of the stresses, depending on the constraints of the ensemble. However, this paper tries to show why it is not only the Boltzmann factor of the points of the phase space that determines the expected distribution in the thermodynamic equilibrium but also the degeneracy of the points. This is precisely due to the existence of different configurations with respective allowed and forbidden regions in the phase space.

2 Revision of elastic energy and force-moment approaches

The elastic energy approach [9] was an attempt of expressing the Edwards' first formalism [1] in terms of elastic potential energy, rather than volume. As a consequence, a theoretical framework based on stresses (or strains) and geometries was developed to explain the expected features of disordered arrangements of jammed granular media.

The thermodynamical formalism was set up starting from the assumption that, in thermodynamic equilibrium, the expected macromechanical behavior of the sample always take the same value. In particular, if the equivalent stiffness of the system were supposed to be the same in all microstates compatible with a macrostate described by external pressure, the elastic potential energy also would be the same in all of them. The ergodic hypothesis would be guaranteed not by averaging samples in time but in cycles of stress and breakage, and consequently, those arrangements in mechanical equilibrium corresponding to global stiffness values different from those expected in thermodynamical equilibrium would be considered as states out of equilibrium.
However, the physical restriction that the whole arrangement should be a solution of the elastic problem was not rigorously imposed in [9]. This was done by first considering limit situations (Voigt and Reuss states) and then integrating over the allowed regions of every configuration and relating the arithmetic average of the stress to the external pressure. Only crystal-like configurations were analyzed.

The force-moment approach [17, 18] properly imposes that the assembly must fit a solution of the elastic problem and can be applied to arrangements with different values of equivalent stiffness and, therefore, of energy. This means

that, if particles are small in comparison with the scale of variation of the macroscopic stress field τ_{ij}, the latter must coincide with the average equivalent stress field over the whole system σ_{ij}. τ_{ij} is the stress field which fits a solution of the elastic problem with average equivalent values of constitutive relationships. In consequence it is possible to set up an ensemble based on the additive force-moment tensor $\Sigma_{ij} = \sigma_{ij} V$, with V being the volume of the system. Then, the Boltzmann factor used in the canonical ensemble depends on a linear function of the stresses, whereas the external control parameter, the tensorial temperature, is fixed by angoricity.

The elastic energy approach showed that consideration of the different configurations and the allowed regions of the phase space can be useful to determine why some configurations are more likely than others and why some of them are barely present. The same methodology, revised and extended to general cases, is followed in this paper, since it is useful for a better definition of the random close packing [19] state or of the maximally random jammed state [20]: if the expected probability of each configuration in equilibrium were known, it would be possible to determine which the expected packing ratio of the sample is. However it is only possible if the constrains of the ensemble are clearly established in a suitable phase space. The objective of this paper is to show up how the nature of the phase space is.

3 Equilibrium and phase space

In this section it is proposed the τ, T phase space (τ, T have been chosen because the Latin word for stress is *tensio*) for those ensembles in which the stress state of the granular system is externally set. Since granular $\aleph$-dimensional systems ($\aleph = 1, 2, 3$) are characterized by both the strong interaction between particles and the inelasticity of collisions, the usual $2\aleph N$-dimensional Γ phase space (described by the position and the momenta (p_i, q_i) of the N grains) together with the complex and dissipative dynamics make it difficult to apply the usual statistical mechanics frameworks. Therefore it is interesting to use a different phase space in order to compare packings and in order to apply statistical analysis.

This is possible by taking advantage from the fact that sometimes granular arrangements must correspond to a solution of a macroscopic elastic problem. This is the case of static, jammed and compressed packings in which the size of the particles is small in comparison with the scale of variation of the macroscopic stress field (for instance, this approach would not be appropriate for diluted granular gases or systems with few particles).

In this way, one possibility is the analysis of the ensemble according to the interaction forces of the particles. It has been done within the framework of the *force network ensemble* theory [14, 15, 16, 12]. Jammed packings are usually

hyperstatic (i.e., the amount of force components is substantially larger than the number of force balance constrains) and they can be compared as a collection of coordinates in a $zN/2$-dimensional phase space, being z the average coordination number. However it was also proved that force balance constraints on every particle reduce the dimension of the space.

Other possibility is the use of the equivalent stress (or force-moment) fields associated to every particle as coordinates of the phase space, instead of forces: every arrangement in mechanical equilibrium with an external stress field can be compared as a collection of points in a stress τ (or force-moment T) phase space, irrespective of where the particles are (in the real space) and which their respective neighbors are. Then it is possible to obtain the most probable distribution of points which satisfies the restrictions of the ensemble (total energy or average equivalent force-moment field). It is being referred to this space as "phase space" in the sense of that it is the space of all possible states of these system but it is very important to emphasize that the laws of classical mechanics are not applicable there.

Before presented in depth which the nature of the τ, T phase space is, some points on the different Boltzmann and Gibbs approaches on the definition of the equilibrium must be clarified [21]. The Boltzmann approach needs to introduce some macroscopic variables (e.g. kinetic energy for ideal gases) and equilibrium is defined by reference to the macrostate, which is uniquely given by a set of values of the macrovariables. Usual restrictions for ideal gases are those given by the microcanonical (N, V, E), canonical (N, V, T) or grand canonical (μ, V, T) ensembles [1]. The expected distribution in the equilibrium is obtained by maximizing the Boltzmann's entropy $S \propto \ln \Omega$ [2], and it gives which the most probable distribution of an ensemble subjected to the same constraints is. The problem is not mechanical but statistical one, because the role of the dynamics is trivial for this definition: it is being compared, among the solutions of a particular physical problem, the class that it is compatible with the macroscopic knowledge of a system.

On the other hand, the starting point for the Gibbs approach is to suppose that the points in the phase space are distributed according to a probability density which is invariant under the flow of dynamics, i.e. this distribution function is a solution of Liouville's equation. Equilibrium is defined for a situation where the probability density function is not an explicit function of time and it becomes a function of the global constants of motion. The statistical mechanical analogues of thermodynamic quantities are either fixed external parameters, related to phase functions or functionals of the density function (e.g. the Gibbs entropy $S \propto \rho \ln \rho$).

[1] V is the volume, E is the energy, T is the temperature and μ is the chemical potential.
[2] Ω is the number of microstates compatible with a macrostate of the system

In the case of ideal gases, both approaches are successful and they give the same expected distribution for the same constraints. Moreover, in these thermal systems particles are in motion so they are changing the coordinates of the phase space as time goes by, but the density function in the equilibrium is invariant. Therefore the ergodic hypothesis is satisfied: the time average of any variable associated to the system coincides to its ensemble average.

However, as the evolution in time of a static packing is not produced by itself, the distribution of the packing in the phase space can only be changed by driving the system (shaking, taping, compressing,...). It gives the opportunity of being unconcerned about whether solutions are steady in time or not or about which the time average of any quantity associated to a packing is. Then, following the Boltzmann approach, it is possible to compare different packings of a static and jammed granular system (microstate) compatible to the same external constraints. An ensemble is considered as a set of copies of the packing that correspond to all different configurations for a given macrostate. Independently of how they had been arranged (i.e. independently of the dynamics during the driving process), they can be identified with a set of points in a suitable phase space. In the absence of further information there is not any a priori reason for favoring one of these microstates more than any other. Hence it should be natural constructing the equilibrium function by assigning equal statistical weights to all the functions compatible with the requirements of the ensemble.

Furthermore, when ideal gases are considered, the distribution function can be analyzed in the phase space of a single particle. But, in the end, this is possible because the Boltzmann factor, i.e. the statistical weight of the points of the phase space, depends on the Hamiltonian function, which is an additive and completely separable function (i.e. $\mathcal{F}(q_1, q_2, \cdots, q_N, p_1, p_2, \cdots, p_N) = \sum_{i=1}^{N} f(q_i, p_i)$). It means that the possibility of using the phase space of one particle just lies in a mathematical feature, but it does not depend on how the mechanical interaction of the particles is. Similarly, approaching solutions of static granular packings compatible to a macroscopic constraint is formally analogous. Both the ensembles reported in section 2 above are also based on additive and separable functions: the total elastic energy and the total force moment of a microstate are equal to the sum of the separate contribution of each particle. Therefore, following the Boltzmann approach and using the τ, T phase space, it is possible to analyze solutions as if the system were decoupled. Respectively, the angoricity and the average elastic energy play the role of the "temperature", the total force-moment tensor or the total elastic potential energy play the role of the "Hamiltonian function". They only depend on the "position" of the particles in the"phase space" (i.e. on coordinates Σ_{ij}^{k} or σ_{ij}^{k}) but they do not depend on the "relative position" of the other particles (i.e. $\Sigma_{ij}^{k} - \Sigma_{ij}^{l}$ or $\sigma_{ij}^{k} - \sigma_{ij}^{l}$). The whole partition function is equal to the partition function of one particle to the power N and the "phase space" of a single particle can be used. So that the number of dimensions of this phase space is small,

$(\aleph+1)\aleph/2$. It is very important to emphasize that this assertion is just based on mathematical arguments. As a result of the mechanical interaction between particles, they can be located in stress or force-moment levels, but for statistical purposes the system is decoupled.

At this point it is possible to analyze how the nature of the phase space of a single particle is. The τ, T phase space has two important features: 1) its accessible region (given by the integration limits of the coordinates and the volume element such as the points within this volume can be compatible with a physical solution of a given problem) and 2) the degeneracy of the points, or density of states (which comes from the capability of geometrical patterns, or configurations, to cover regions of the phase space). Both these issues are analyzed below together with an explanation for why using a change of variables can be interesting.

4 Coordinates (p, q, ω) and (P, Q, Ω)

If the ensemble is based on the total elastic potential energy of the granular system, a natural workshop is provided by the components of the stress tensor σ_{ij} [9]. In the static case, for elastic continuum media the energy density is given by

$$e = \frac{dE}{dV} = \frac{1}{2}\sigma_{ij} S_{ijkl} \sigma_{kl}, \tag{1}$$

where S_{ijkl} is the compliance tensor of the material.

Within granular media the particles are in equilibrium under a finite number of forces. If they are elastic, they store elastic potential energy, which for a particle k is given by

$$E^k = \frac{1}{2}\int_{V^k} \bar{\sigma}^k_{ij} \bar{S}^k_{ijmn} \bar{\sigma}^k_{mn} dV^k = \frac{1}{2}\int_{V^k_{\mathrm{P}}} \sigma^k_{ij} S^k_{ijmn} \sigma^k_{mn} dV^k_{\mathrm{P}} \simeq \frac{1}{2}\left(\frac{1}{2}\sum_l \frac{f^{kl}}{K_{\mathrm{D}}}\right), \tag{2}$$

where σ^k_{ij} is the actual stress field within the volume of the particle V^k_{P}, S^k_{ijmn} is the compliance tensor of the material, $\bar{\sigma}^k_{ij}$ is the stress field averaged not only over the volume of the particle but also on the associated void (i.e., over the respective Voronoi cell V^k), and $\bar{S}^k_{ijmn}$ is the equivalent compliance tensor. f^{kl} are the interacting forces[3] and K_{D} is the stiffness of the particles (i.e., the ratio between the applied force and the reduction of the diameter).

In order to translate a set of forces into an equivalent average stress field the

[3]The final equality of the expression is only for linear force–displacement relationships, e.g., elastic disks.

average stress tensor [22] can be used:

$$\bar{\sigma}_{ij}^k = \frac{1}{V^k}\int_{V^k} \sigma_{ij}^k dV^k = \frac{1}{V^k}\sum_l r_i^{kl} f_j^{kl}, \tag{3}$$

where r^{kl} is the position of the point of application of the force f^{kl}.

According to the possible arrangements, some set of forces can be equivalent to the same stress field. Therefore, the phase space determined by $\bar{\sigma}_{ij}$ is a good workshop to compare microstates, and according to the value of the forces it is possible to calculate the elastic potential energy. This is the τ phase space.

Nevertheless, the nature of these media makes it preferable to use other stress state variables. For the case of 2D media, considering the invariants of the second-order stress tensor $\bar{\sigma}_{ij}$, the variables (p, q, ω), $(\sigma_{\mathrm{I}}, \sigma_{\mathrm{II}}, \omega)$, or (σ, m, ω) are more suitable.

The coordinates p, q, ω are based on Mohr's circle and are defined as

$$p = \frac{\bar{\sigma}_{xx} + \bar{\sigma}_{yy}}{2} = \frac{I_1}{2}, \tag{4}$$

$$q = \left[\left(\frac{\bar{\sigma}_{yy} - \bar{\sigma}_{xx}}{2}\right)^2 + \bar{\sigma}_{xy}^2\right]^{\frac{1}{2}} = \left[\frac{1}{4}I_1^2 - I_2\right]^{\frac{1}{2}}, \tag{5}$$

$$\omega = \frac{1}{2}\arctan\frac{2\bar{\sigma}_{xy}}{\bar{\sigma}_{yy} - \bar{\sigma}_{xx}}. \tag{6}$$

p and q[4] (or $q' = q/p$), the centrum and radius of Mohr's circle, relate to the invariants $I_1 = \bar{\sigma}_{ii}$ and $I_2 = \epsilon_{ij}\bar{\sigma}_{xi}\bar{\sigma}_{yj}$ of the Cauchy stress tensor (being ϵ_{ij} the Levi-Civita symbol); therefore, they are also independent of the reference system. However, ω depends precisely on the orientation of the principal directions of the tensor. Other alternatives are to use the principal stresses σ_{I} and σ_{II} (also invariants) together with ω, or the minor principal stress σ and the anisotropy factor m (the ratio between both stresses $m = \sigma_{\mathrm{I}}/\sigma_{\mathrm{II}}$).

Using these coordinates rather than the components of the Cauchy stress tensor is interesting because some physical restrictions and some magnitudes are conveniently expressed as functions of them; for instance, the elastic potential energy of an isotropic continuum medium does not depend on ω, but it often does when the medium is not isotropic (e.g., a particulate medium).
In this paper, (p, q', ω) are used for the stress phase space. In short, they express the stress level, the relative deviatoric component of the stress state, and the orientation, respectively.

[4]This notation of stress as p, q is widely used in triaxial tests performed in soil mechanics. Obviously they are not the position and momentum in the Γ phase space.

The volume of the accessible region of the τ phase space of one particle $\mathcal{V}_\tau$ can be expressed as

$$\mathcal{V}_\tau = \int_0^\infty \int_0^\infty \int_{-\sqrt{\bar{\sigma}_{xx}\bar{\sigma}_{yy}}}^{\sqrt{\bar{\sigma}_{xx}\bar{\sigma}_{yy}}} d\bar{\sigma}_{xx} d\bar{\sigma}_{yy} d\bar{\sigma}_{xy} = \int_0^\infty \int_0^1 \int_0^{2\pi} 2p^2 q' dp dq' d\omega. \quad (7)$$

The integration limits [5] are those which guarantee that, for any state, the respective principal stresses are positive. It means that the stress field is compressive in any spatial direction (as it is expected for cohesionless materials). The principal stresses are the eigenvalues of the Cauchy stress tensor and, according to the characteristic equation, both of them are positive when $\bar{\sigma}_{xy}^2 \leq \bar{\sigma}_{xx}\bar{\sigma}_{yy}$.

On the other hand, the force-moment approach is based on the force-moment tensor $\Sigma_{ij}^k = \bar{\sigma}_{ij}^k V^k = \sum_l r_i^{kl} f_j^{kl}$. For a system of N particles, the total Σ_{ij} is given by the sum of the force-moment tensor of every particle $\Sigma_{ij} = \sum_k \Sigma_{ij}^k$. Therefore, the coordinates of the phase space can be directly Σ_{ij}. It is being referred herein to this space as the T phase space.

However, according to the invariants of Σ_{ij}, it is also possible to define the coordinates P, Q, Ω as $P = \hat{I}_1/2$, $Q = \sqrt{(1/4)\hat{I}_1^2 - \hat{I}_2}$, and $\Omega = (1/2)\arctan\frac{2\Sigma_{xy}}{\Sigma_{yy}-\Sigma_{xx}}$, being $\hat{I}_1 = \Sigma_{ii}$ and $\hat{I}_2 = \epsilon_{ij}\Sigma_{xi}\Sigma_{yj}$ the invariants of Σ_{ij}. Q' is again the relative deviatoric component, $Q' = Q/P$, and ϵ_{ij} the Levi-Civita symbol.

In this paper, (P, Q', Ω) are proposed for the force-moment phase space. The integration limits and the volume element are similar to those used above: $P \in [0, \infty)$, $Q' \in [0, 1]$, $\Omega \in [0, 2\pi)$ and $d\mathcal{V}_\mathrm{T} = 2P^2 Q' dP dQ' d\Omega$.

5 Canonical ensembles

Consider the case in which the average external stress field is kept constant, although the system is driven many times to make it reach the equilibrium. The system is supposed to be in contact with an external pressure bath.

Following the approach of elastic potential energy, the expected statistical weight of a configuration in equilibrium would be governed by a Boltzmann factor which depends on quadratic functions of the stresses as

$$e^{-\frac{E_{\alpha,(p^2,q'^2,\omega)}}{\beta}}, \quad (8)$$

[5] Actually, ω should be evaluated within the interval $[0, \pi)$, because the stress states of ω and $\omega + \pi$ are the same. Nevertheless, this doubled evaluation results in a more intuitive representation. Note that, in this way, a determined system of forces, equivalent to a stress field, would be represented by two symmetrical points in the phase space.

where β relates to the external pressure and the expected equivalent stiffness of the system, and the energy depends on the configuration and on the stresses. This approach does not mean that the energy is constant during the driving process, but that, once the kinetic energy has been dissipated and the packing is again in mechanical equilibrium with the external pressure, the elastic energy of the ensemble is the same that it was before the driving. As the energies can be expressed as $E_\alpha = p^2 \cdot \hat{M}_{\alpha(q'^2,\omega)}$ (see [9], although the function was expressed in terms of other variables $E_\alpha = E_{I(K_D,\sigma^2)} M_{\alpha(m,\omega)}$), the probability of the configurations actually depends on the functions $\hat{M}_{\alpha(q'^2,\omega)}$[6]. The energy increases with the stress level and with the anisotropy factor, so the statistical weight decays. After imposing the restrictions of this approach, the following important conclusion is obtained: the probability of the configurations depends strongly on the volume of the respective allowed regions. This consideration can be useful for other approaches.

On the other hand, following the force-moment approach, the Boltzmann factor would depend on the force-moment tensor [10, 11, 17, 18] as

$$e^{-\chi_{ij}\Sigma_{ij}}, \tag{9}$$

where χ_{ij} is the angoricity, a second-order tensor. Using a reference system x, y according to the principal directions of the angoricity, i.e., those in which $\chi_{xy} = 0$, the statistical weight does not depend on Σ_{xy}.

The physical meaning of the angoricity can be deduced by obtaining average values. For instance, by integrating over the volume of the T phase space of a single particle (analogous of Eq. 7 for Σ_{ij} variables, instead of $\bar{\sigma}_{ij}$), it is obtained that the expected value of Σ_{xx} is given by:

$$< \Sigma_{xx} >= \frac{\Sigma_{xx}}{N} = \frac{\int_0^\infty \Sigma_{xx}^{3/2} e^{-\Sigma_{xx}\chi_{xx}} d\Sigma_{xx}}{\int_0^\infty \Sigma_{xx}^{1/2} e^{-\Sigma_{xx}\chi_{xx}} d\Sigma_{xx}} = \frac{3}{2}\frac{1}{\chi_{xx}} \tag{10}$$

The 3/2 and 1/2 powers on Σ_{xx} come from the integration limits of Σ_{xy} ($\Sigma_{xy} \in (-\sqrt{\Sigma_{xx}\Sigma_{yy}}, +\sqrt{\Sigma_{xx}\Sigma_{yy}})$).
Acting in the same way, $< \Sigma_{yy} >= (3/2)(1/\chi_{yy})$ and $< \Sigma_{xy} >= 0$. Using $\Sigma_{ij} = V\sigma_{ij}$ and $\sigma_{ij} = \tau_{ij}$ it is shown that χ_{ij} is actually 3/2 of the inverse of the average external force-moment tensor $V\tau_{ij}$ per particle, i.e.,

$$\chi_{ij} = \frac{3}{2}\frac{N}{V}\left(\tau_{ij}\right)^{-1}, \tag{11}$$

where V is the volume of the whole system.

However, the exponent of the Boltzmann factor can also be expressed as

$$\chi_{ij}\Sigma_{ij} = P\chi_P\left[1 + Q'\cos 2\Omega\chi_{Q'\Omega}\right], \tag{12}$$

[6]The reference system is established according to the orientation of the configuration, so that ω refers here to the angle of the principal stresses with respect to the configuration.

where $\chi_P = (\chi_{xx} + \chi_{yy})$ and $\chi_{Q'\Omega} = (\chi_{yy} - \chi_{xx})/(\chi_{yy} + \chi_{xx}) \in [0, 1)$. The advantage of writing the Boltzmann factor in this way is that, in the statistical weight of each point of phase space, it separates the contribution due to the force-stress level P from the contribution due to the relative deviatoric component Q' and the orientation Ω, depending on the external control parameters χ_P and $\chi_{Q'\Omega}$.

As some physical restrictions are independent of the stress level, it is interesting to consider the distribution of points in Q', Ω planes, for any value of P or for all of them. The integration of the points over all the values of P and its representation over a polar Q', Ω plane is referred to as the *comparison plane* (i.e. a plot which displays $Q' \sin \Omega$ as ordinate plotted against $Q' \cos \Omega$ as abscissa) [7].

If every point in the T phase space of a single particle is supposed to have the same multiplicity, the partition function (when negative stresses are not allowed) is given by

$$Z_{\mathrm{T}}(1, \chi_P, \chi_{Q'\Omega}) = 2 \int_0^\infty \int_0^1 \int_0^{2\pi} e^{-\chi_P P(1+\chi_{Q'\Omega} Q' cos 2\Omega)} P^2 Q' dP dQ' d\Omega. \quad (13)$$

Integrating over all the values of P leads to the expected density in the comparison plane $\rho_{(Q',\Omega)}$, which just depends on $\chi_{Q',\Omega}$.

For the case of isotropic compression, $\chi_{xx} = \chi_{yy} = \chi_P/2$, so that the exponent of the Boltzmann factor just depends on P, i.e., $\chi_{ij}\Sigma_{ij} = P\chi_P$. This means that, if the granular system is in equilibrium with an external isotropic stress field, the probability of the particles in the ensemble will not depend on either Q' or Ω, so that the expected statistical distribution of particles according to their respective values of P will be

$$\rho_{\mathrm{T}(P)} = \frac{\chi_P^3}{2} e^{-\chi_P P}, \quad (14)$$

satisfying $\int_0^\infty \rho_{\mathrm{T}(P)} P^2 dP = 1.0$. Note that the volume element is $d\mathcal{V}_{\mathrm{T}P} = P^2 dP$ and it affects the expected number of particles n_{P} in each $P \pm \Delta P/2$ interval:

$$\frac{n_{\mathrm{P}}}{N} = \frac{\chi_P^3}{2} e^{-\chi_P P} P^2 \Delta P \quad (15)$$

Moreover, integrating over P, in the isotropic compression case every point in the comparison plane is supposed to be equally likely to be found

$$\rho_{\mathrm{T}(Q',\Omega)} = \frac{1}{\pi}, \quad (16)$$

satisfying $\int_0^1 \int_0^{2\pi} \rho_{\mathrm{T}(Q',\Omega)} Q' dQ' d\Omega = 1.0$.

[7] In a $\bar{\sigma}_{ij}$ phase space, the comparison plane plots the polar distribution of q' and ω, integrated for all p values.

On the other hand, for anisotropic stress fields, the higher the anisotropy ratio, the stronger the dependence of the Boltzmann factor on Q' and Ω. This is shown in Fig. 1, where it is plotted for different values of $\chi_{Q'\Omega}$ and P. As Ω is fixed according to the principal directions of the external stress field (via the angoricity), the expected local stress fields are not isotropically oriented but according to some prevailing directions.

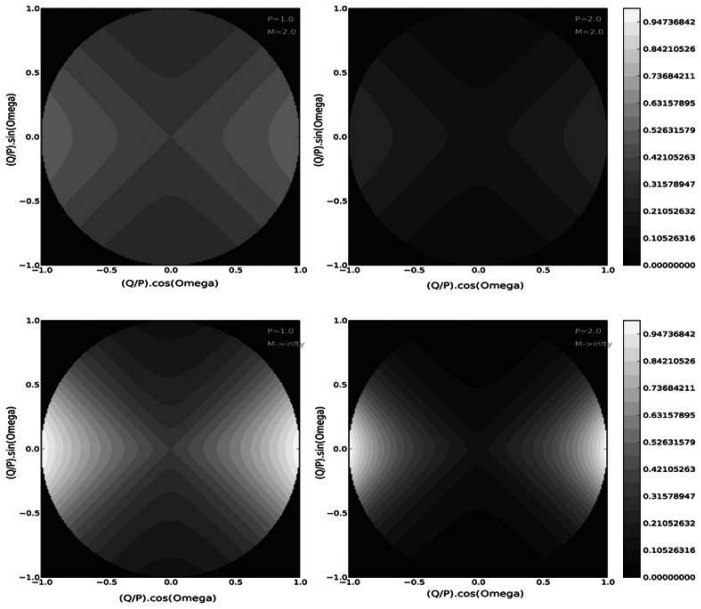

Figure 1: Representation of the Boltzmann factor (using Eqs. 9 and 12) over two constant-P planes according to the force-moment approach. $\chi_P = 1.0$. The higher the P, the smaller the value of the Boltzmann factor, whereas $\chi_{Q'\Omega}$ sets the dependence on Q' and Ω. (a) $P = 1.0$ and $\chi_{Q'\Omega} = 0.33$, (b) $P = 1.0$ and $\chi_{Q'\Omega} = 1.0$, (c) $P = 2.0$ and $\chi_{Q'\Omega} = 0.33$, and (d) $P = 2.0$ and $\chi_{Q'\Omega} = 1.0$. If $\chi_{Q'\Omega}$ is 0.0 (meaning that the external stress is isotropic), every point within any constant-P plane is equally likely to be filled and uniform gray circles are expected.

6 Configurations. Allowed and forbidden regions

6.1 The degeneracy of the points in the phase space

Irrespective of which canonical ensemble is used, it is highly relevant that some points of the stress phase space can be filled by several configurations (and sometimes with several orientations and several internal degrees of freedom) while other points are forbidden for some of the configurations. Consequently, the phase space must be characterized by a density of states function which comes from the sum of the allowed regions of all configurations in all possible orientations with respect to the principal directions of the external pressure. Then, Eq. 13 becomes

$$Z_{\mathrm{T}}(1,\chi_P,\chi_{Q'\Omega}) = \int_0^{\infty}\int_0^{1}\int_0^{2\pi} g_{(Q')}e^{\chi_P P[1+\chi_{Q'\Omega}Q' cos2\Omega]}2P^2Q'dPdQ'd\Omega, \tag{17}$$

where $g_{(Q')}$ is the total density of states function, which is supposed to be independent of both Ω and P.

Since this function is actually equal to the sum of the respective contribution of every configuration $g_{\alpha(Q')}$, it is also possible to express the partition function as

$$Z_{\mathrm{T}}(1,\chi_P,\chi_{Q'\Omega}) = \sum_{\alpha}\int_0^{\infty}\int_0^{1}\int_0^{2\pi} g_{\alpha(Q')}e^{\chi_P P[1+\chi_{Q'\Omega}Q' cos2\Omega]}2P^2Q'dPdQ'd\Omega. \tag{18}$$

The functions $g_{\alpha(Q')}$ are equal to 0 within the respective forbidden regions but can take a normalized value within allowed regions (because some configurations could have also internal degeneracy). Expressing the partition function in this way reflects exactly not only the stress state in which particles of every microstate are located but also the configuration to which they belong. Then, some expected properties, especially the associated packing ratio, can be directly measured if the distribution function is separable in configurations.

6.2 Physical reasons for allowed and forbidden regions

Packing spheres is inherently a geometrical problem due to exclusion-volume effects, and how particles can locally be arranged affects the expected distribution of the disordered total arrangement. Two conceptual approaches for the study of jammed packings have emerged: the "ensemble" aproach and the "geometric-structure" approach [23]. The elastic energy approach [9] includes features of both approaches, by considering the mechanical stability of geometrically compatible local packings within an ensemble. This procedure is also

followed herein.

A configuration α refers [9] to a fixed number of particles arranged in a specific geometrical pattern such that the cluster is in equilibrium with the stress field. In this way, some crystal-like configurations can be analyzed. However, there are other possibilities for the definition of the configuration. In this work, they are distinguished according to the number of forces.

The number of degrees of freedom and their stability determine the allowed region of the phase space, which depends on the kind of interaction between the particles and on the geometric compatibilities. An important advantage of using the coordinates (P, Q', Ω) is that these physical restrictions are independent of the force-moment level (the ability of a configuration to fill a point only depends on Q' and Ω), so that the comparison plane can also be used to analyze the size and shape of the respective allowed region.

To illustrate this assertion, the simplest case of a 2D frictionless monodisperse system is analyzed. In this medium, only five configurations are possible, defined respectively by the number of forces L: 6, 5, 4, 3, and 2. The forces f^{kl} acting on the particle are ordered according to the angle θ^{kl} with respect to a fixed reference system associated with the configuration. There are three kind of restrictions:

- Restrictions due to the kind of interaction
  In cohesionless materials, all forces must be positive:
  $$\forall k, l \; f^{kl} \geq 0. \tag{19}$$

- Restrictions due to mechanical equilibrium
  In 2D there are just two restrictions:
  $$\forall k \sum_{l} f_i^{kl} = 0. \tag{20}$$
  As there is no friction, all forces are central, and there are no moments.

- Restrictions due to geometrical incompatibilities
  For a 2D monodisperse system the maximum number of forces is six, and there are also some geometrical restrictions:
  $$\forall k, l \; \theta^{kl} - \theta^{kl-1} \geq \pi/3 \tag{21}$$
  and one equation
  $$\forall k \sum_{l} = \Delta\theta^{kl} = 2\pi, \tag{22}$$
  with $\theta^{k0} = \theta^{kL} - 2\pi$.

As a result, every configuration has an internal number of degrees of freedom with bounded values of the respective coordinates. All these restrictions are independent of the force scale (if the forces are increased by K times, restrictions given by Eqs. 19, 20, 21, and 22 are still satisfied), and in any constant-P plane the allowed regions extend over the same Q', Ω values. So, it is not necessary to analyze the whole volume of the phase space, but just the comparison plane. Irrespective of the configuration, if the force-moment state approach is followed, every allowed point has the same statistical weight, whereas following the elastic energy approach it depends on the value of the forces.

Then, the respective $g_{\alpha(Q')}$ of a configuration is equal to the normalized integration over all possible orientations of the geometrical patterns with respect to the principal stresses (fixed by the principal directions of the angoricity). These functions include the features of the particles (size distribution, shape, roughness, strength, etc.) because this determines which configurations are possible and which regions of the phase space are covered.

7 Probability of configurations and transitions

Although not only the statistical weight but also the density of states affect the expected statistical distribution, probably particles are not totally free to move between configurations, and not all transitions are likely to occur during any cyclic process. As a result, the expected state after a protocol could relate to a Markov process, determined by the allowed regions. This could explain why, for instance, in 2D monodisperse media, protocols often cause most of the particles to arrange according to the *six-force* configuration, although other configurations may also be expected (because they also have considerable allowed areas)

So, consider a particle in equilibrium with some forces (i.e., belonging to a configuration) in a system of N particles. If the external conditions of the whole system (i.e., the angoricity) are modified, another solution of the elastic problem with a different arrangement could be achieved. During this process, the forces on the particle can change, and it is possible to draw its path in the phase space. If this path remains within the allowed region, the particle can be kept in the same configuration. The particle could also change into other configurations without breaking if they overlap. Finally, if the stress path reaches a region where the configuration is not possible, it will break locally. Once this happens, the particle could fall into any configuration, according to the probability of each.

As a consequence, the stochastic evolution of the system in a determined driving process could be supposed to be a Markov chain in which the probability of a particle belonging to a configuration α in the $(N+1)$th step P_α^{N+1} depends on the distribution in the current step N and on the transition proba-

bilities $p_{\alpha\beta}$. These could be associated with the features of the allowed regions of the configurations. If the probability of changing the stress stress is p_1, the probability of breaking is $p_{2\alpha}$, the probability of changing to overlapping configurations is $p_{3\alpha\beta}$, and the probability of falling into a configuration once the equilibrium has been broken is $p_{0\alpha}$, it follows that

$$P_{\alpha}^{N+1} = p_{\alpha\beta} P_{\beta}^{N}, \tag{23}$$

where

$$p_{\alpha\alpha} = (1 - p_1) + p_1 \cdot (1 - p_{2\alpha}) \cdot (1 - p_{3\alpha\beta}) + p_1 \cdot p_{2\alpha} \cdot p_{0\alpha} \tag{24}$$

and

$$p_{\alpha\beta} = p_1 \cdot (1 - p_{2\beta}) \cdot p_{3\alpha\beta} + p_1 \cdot p_{2\beta} \cdot p_{0\alpha}. \tag{25}$$

The probability of changing the stress state P_1 would depend on the cyclic modification of the external control parameters, and this could explain the reported strong dependency on the protocol. The probability of falling into a configuration $P_{\alpha 0}$ could relate to the size of the allowed region on the comparison plane, whereas the probability of breaking $P_{2\alpha}$ could relate to the shape of the region.

8 Qualitative analysis of a 2D monodisperse system

8.1 Configurations and allowed regions

The possible equilibrium configurations of a 2D monodisperse granular system have been analyzed. This was done by numerically generating combinations of forces and angles which maintain the equilibrium and which correspond to the same value of P ($P = 1.0$). Then, points were plotted on the comparison plane.

The surveying of combinations was done by fixing the angles of each of the analyzed configurations and then taking possible values of some of the forces within the bounded interval. The number of variables depends on the number of degrees of freedom of the configuration. The domain of the variables was divided into a uniform grid, according to a fixed interval, and the other forces were obtained by applying the restrictions of force balance. The resulting groups which included negative forces were automatically discarded. The value of $P = 1.0$ was imposing just by adding one restriction more. This is not necessary but it saves computation time because it avoids considering groups of forces which are actually scalar transformation each other (they would be plotted at the same point in a polar representation of (Q', Ω)). The interval of the grid was taken with values of different orders of magnitude, and although the number of obtained points was obviously increased with smaller intervals, it was observed that all the points were always located within the same region. Moreover, when the elastic energy approach was set up [9] the boundaries of

the *six-force* configuration were analytically obtained (although other variables were used in that paper) and that procedure gave the same result. Some configurations analyzed in this way are presented.

The *six-force* configuration has five degrees of freedom (four forces and one angle) because inequalities of angles (Eq. 21) become equalities. So, once the angle is fixed with respect to a reference system, it is possible to analyze which combinations of positive forces keeping the equilibrium are possible. Plotting all these points over the comparison plane reveals the allowed area of this configuration (Fig. 2). It is a key factor that there are three orientations with respect to the principal directions of the equivalent stress field in which Q' can take any value between 0.0 and 1.0. This is absolutely the most stable configuration.

The *five-force* configuration has eight degrees of freedom (three forces and five angles), although angles are strongly bounded due to the inequalities. It is not clear if every combination of angles can be considered as an independent configuration, because the multiplicity of some (Q', Ω) points would be too high. In any case, some representative cases are plotted in Figs. 3, 4, 5, and 6. It is important to realize that there are only points with high values of Q' for a few geometrical patterns. Indeed, the highest value of $Q' = 1.0$ is obtained precisely in the quasihexagonal arrangement (which coincides with a *six-force* configuration in which one force is null). Moreover, the shape of some areas makes it reasonable to consider that the probability of breaking this configurations is very high.

The *four-force* configuration has six degrees of freedom (two forces and four angles). Angles are somewhat less bound than in the *five-force* case. Some combinations can cover high values of Q, but only over a narrow area (indeed, only some lines), so that this configuration is in general quite unstable. Again, it is not clear whether the angles can change without breaking, which would extend the stability area of the configuration. This idea was used in a previous paper [9], where it was supposed that a transition between rhombic configurations happens until the system reaches a totally forbidden area. The result would be a four-pointed star area, covering some high values of Q.

8.2 Numerical simulations

Two different numerical molecular dynamics simulations were performed to qualitatively analyze the distribution in the τ, T phase space. The purpose of these simulations was checking whether, at different stages of the compression process, the distribution of the points on the comparison plane is affected by the allowed regions of configurations or not. However the macroscopic constraints of the ensembles explained above are not totally imposed, because it is much more easy to perform simulations in which the displacement of the walls or the external pressure are controlled, rather than the force-moment or the final elastic energy of the packing. Nevertheless, as it is not being measured neither the

entropy nor the ensemble average of any quantity, these simulations are valid for the objectives of this paper. In addition, after a cyclic compression schedule, if the variation of the volume of the sample is small, then the constraints of the force-moment ensemble are closely matched.

The LAMMPS code, a parallel particle simulator developed at Sandia National Laboratory [24] was used (including the GRANULAR package). The systems consisted of 900 (30×30) and $4,900$ (70×70) frictionless disks [8], which interacted via a viscous and linear (Hookean) contact law (i.e. $\mathbf{F}^{kl} = (K_{\mathrm{H}}\delta - \gamma\frac{m}{2}\dot{\delta})\mathbf{n}^{kl}$, being δ the overlapping between particles k and l). A normal damping coefficient $\gamma \simeq 2\sqrt{2}\sqrt{K_{\mathrm{H}}/m}$ was used in order to dissipate the kinetic energy and compare static solutions. Particles were initially arranged according to a regular square lattice. Some irregular walls were also generated, two of which were fixed while the others were subject to controlled motion or applied force. The compression schedule is described by a first isotropic compression stage and then some anisotropic compression cycles. The sole purpose of the irregularity of the walls was to avoid the whole crystallization of the sample. These walls were generated by locating particles in consecutive contact and in such a way that they separate from the average position of the wall according to a normal distribution. Both the duration of the isotropic compression stage and the period of the cycles of compression Δt were chosen in such a way that $\Delta t/t_{\mathrm{c}} \sim 10^4$, being t_{c} the characteristic time $t_{\mathrm{c}} = \sqrt{m/K_{\mathrm{H}}}$. In the case of 900 particles, an external pressure of $p/K_{\mathrm{H}} \sim 10^{-3}$ was applied (p is given in units of force per unit of length) whereas in the sample of $4,900$ particles a displacement of the walls of $\Delta L \simeq 0.07 L_0$ was imposed (being $L_0 \sim 70 \times D$ and D the diameter).

Fig. 7 and Fig. 9 show the aspect of the granular packings, and Fig. 8 and Fig. 10 show how the respective population density on the comparison plane of the two simulations was. In the first case, this measure was taken after 4 anisotropic compression cycles whereas in the second case it was taken at the end of the isotropic compression stage. The first conclusion is that, although it is an isotropic compression state, the points are not uniformly distributed within the circle as expected for an isotropic compression state, providing evidence that the Boltzmann factor is not the only parameter which determines it (at least if the force-moment approach is followed, because results show that, the lower the value of Q', the higher the density of points). Therefore, the density of states $g_{(Q')}$ strongly determines the expected distribution of particles in force-moment levels.

The number of points obtained in these simulations is not enough to ensure thermodynamic limit conditions. Therefore, obtaining histograms (which would be necessary to know how the $g_{\alpha(Q')}$ functions are and how the distribution de-

[8] Spheres were actually used, instead of disks, in a $2D$ system. Nevertheless, some precautions were taken in order to assimilate this system to a real bidimensional system.

pends on the protocol) it is not still possible. Nevertheless, this plot shows how the allowed regions have a strong influence on the statistical distribution. It is quite interesting that many of the particles are precisely located at the boundaries of the allowed and forbidden regions of the main *six-force* arrangement.

9 Conclusions

It is possible to compare different packings of a granular system compatible to the same external constraints, in a suitable phase space which considers the equivalent stress field $\bar{\sigma}_{ij}^k$ or the force-moment tensor of the particles Σ_{ij}^k. The accessible region of the phase space depends on the nature of the granular system.

According to the scale invariance of the mechanical restrictions, for 2D systems it is not necessary to analyze the whole one-particle phase space but just the P distribution and the area in the comparison plane [polar representation of (Q', Ω) for all P].

Due to the nature of the equilibrium states in particles, some regions are allowed whereas others are forbidden, meaning that some points of the phase space are degenerate. It can be expressed as a density of states function.

The size and shape of the allowed regions of every configuration depend on the degrees of freedom and on the geometrical incompatibilities, mechanical constraints, and the kind of interaction between the particles.

The statistical weight of the points in the phase space is fixed by the ensemble. Nevertheless, the final statistical distribution is strongly affected by the density of states, what is explained according to the allowed and forbidden regions of configurations. The intrinsic properties of the medium, i.e., the features of the particles (size distribution, shape, roughness, etc.), determine these functions, whereas the external stress state fixes the angoricity or the elastic energy (the parameter controlling the statistical distribution). More research is needed to analyze $g_{(Q')}$ and how it can be separated according to the respective contributions of the different configurations $g_{\alpha(Q')}$.

As granular systems do not tend to equilibrium by themselves, it is necessary to drive them. The kind of modifications applied determines the probability for a particle to modify its stress state and thereby transition between configurations. These probabilities could be related to the shape and size of the allowed regions.

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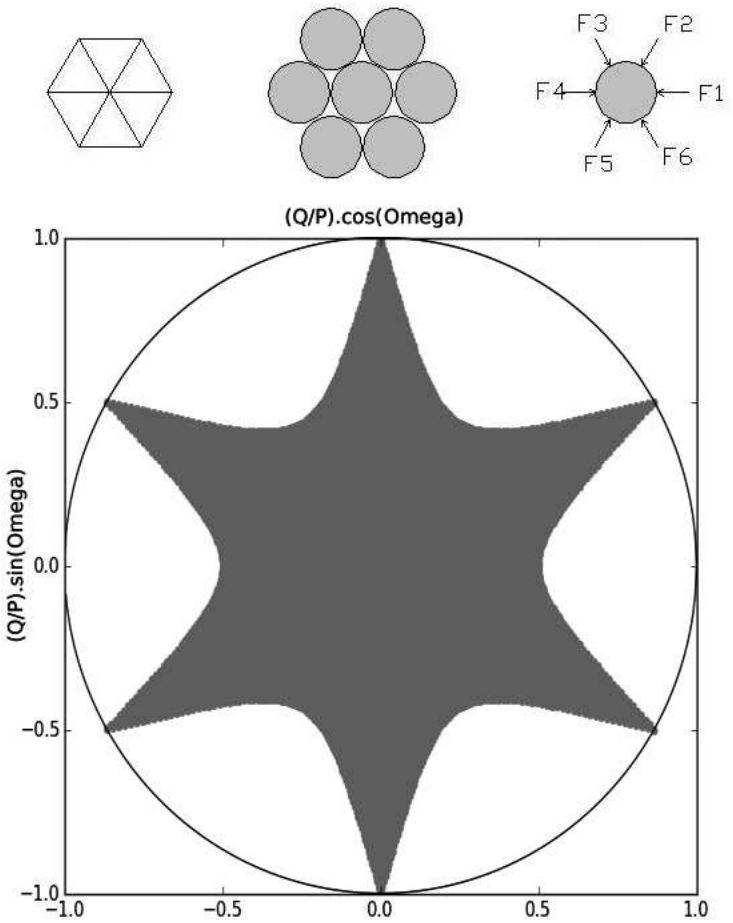

Figure 2: Allowed area of a *six-force* configuration. The only possible combination of angles corresponds to a regular hexagon. This is the configuration which covers the largest area in the constant-P plane. It is about 55% of the expected maximum volume (the circle, which corresponds to an ideal, infinite-strength continuum medium). The highest value of Q which can be resisted in six directions is P, and some wide areas of high values of Q are also covered

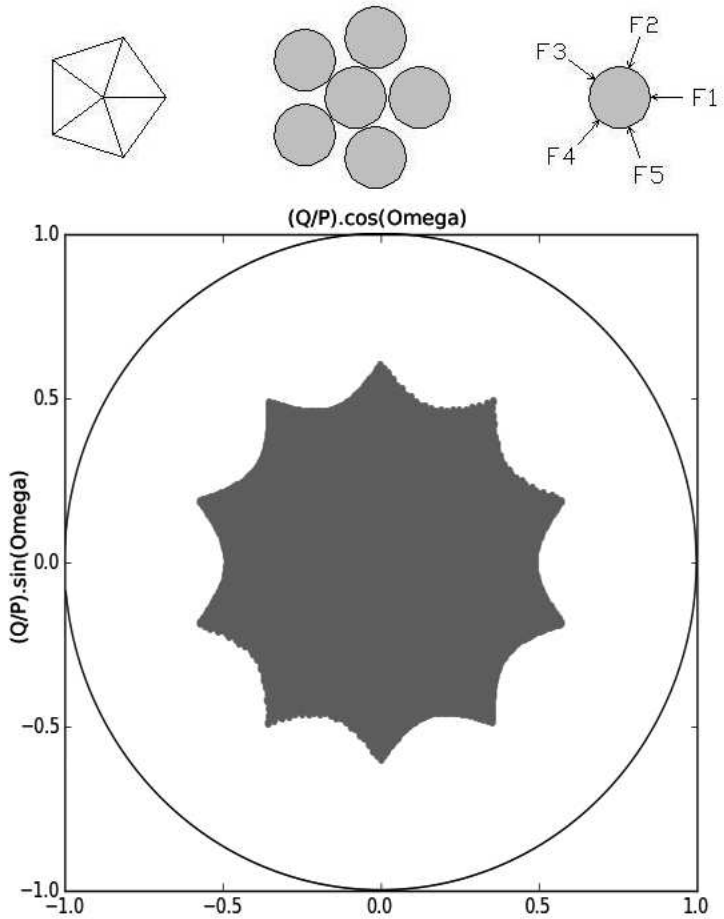

Figure 3: Allowed area of a *five-force* configuration with pentagonal orientation of forces. The area is quite isotropic, and its size is about 32% of the expected maximum volume. The highest value of Q which can be resisted in five directions is less than $0.6P$

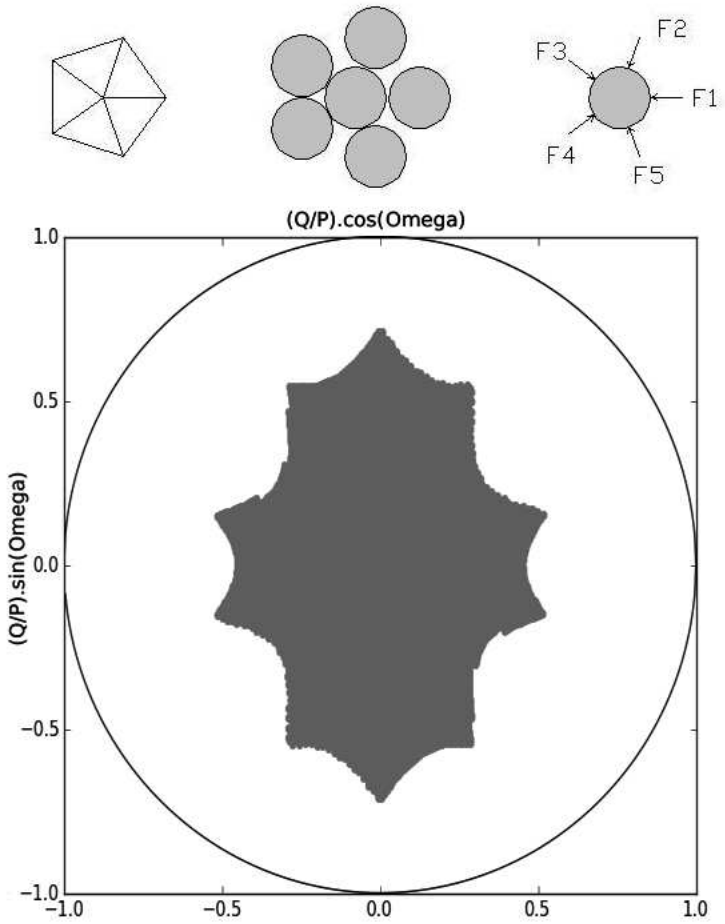

Figure 4: Allowed area of a *five-force* configuration with a slightly modified pentagonal orientation of forces. The area is slightly more anisotropic than in the regular pentagonal case. The size is about 31% of the expected maximum volume, and the maximum value of Q is higher than the regular case in just one direction

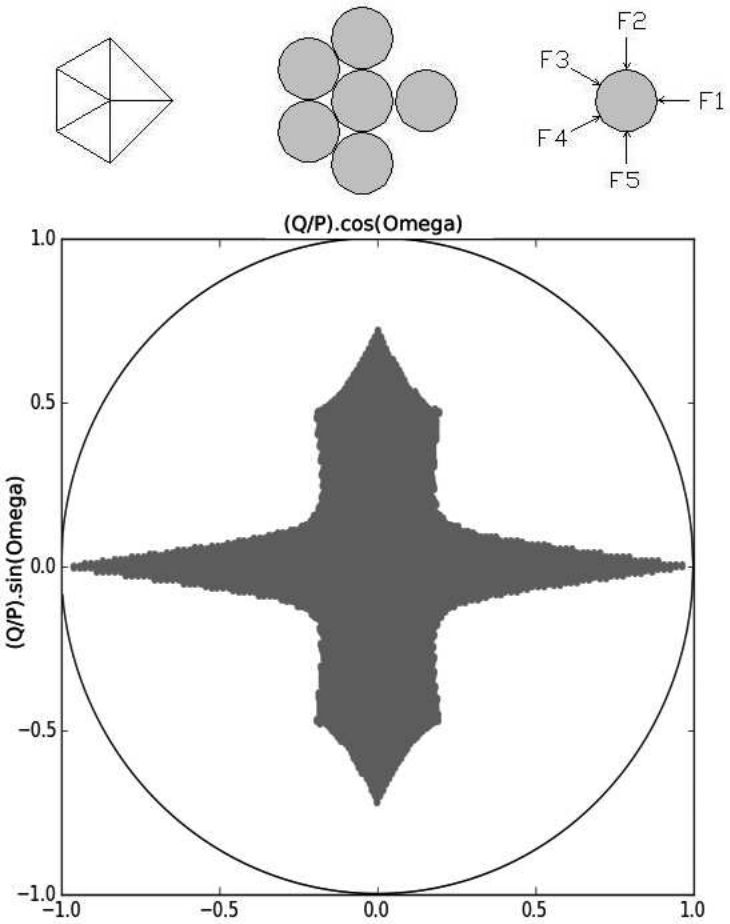

Figure 5: Allowed area of a mixed hexagonal–square configuration. This *five-force* configuration is usually found in the grain boundary of crystalline regions. The size is about 24% of the expected maximum volume, and the highest value of Q is again P, being possible in only one direction

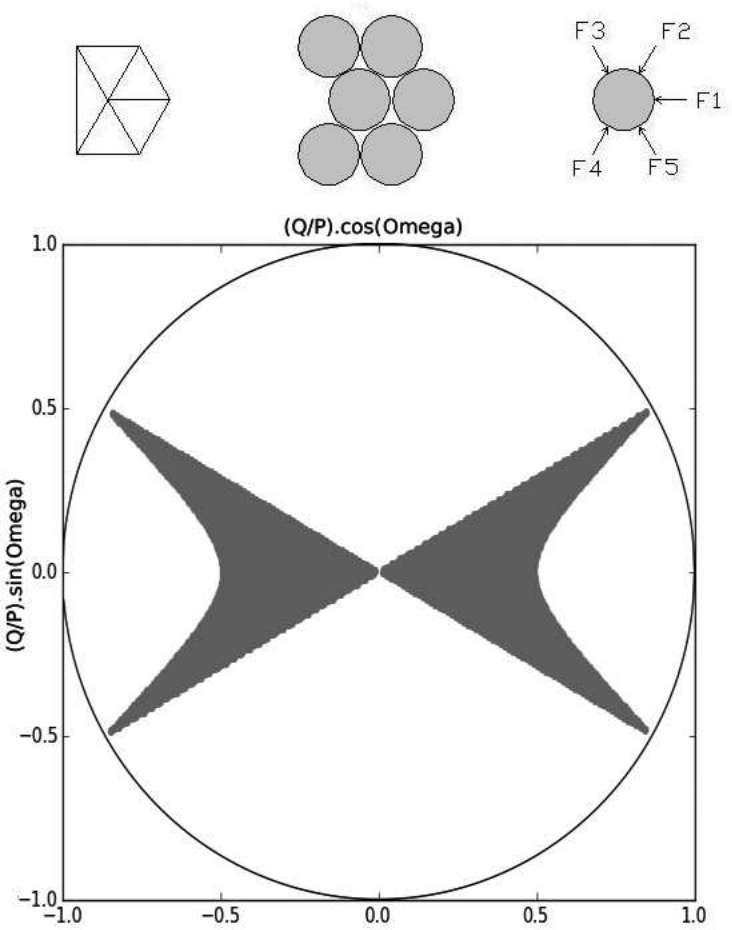

Figure 6: Allowed area of a quasihexagonal *five-force* configuration, being equivalent to a *six-force* configuration in which one force is zero. The size is about 19% of the expected maximum volume, and the highest value of Q is P. However, it is possible in just two directions. As the shape is narrow and strongly anisotropic, this configuration is supposed to be quite unstable

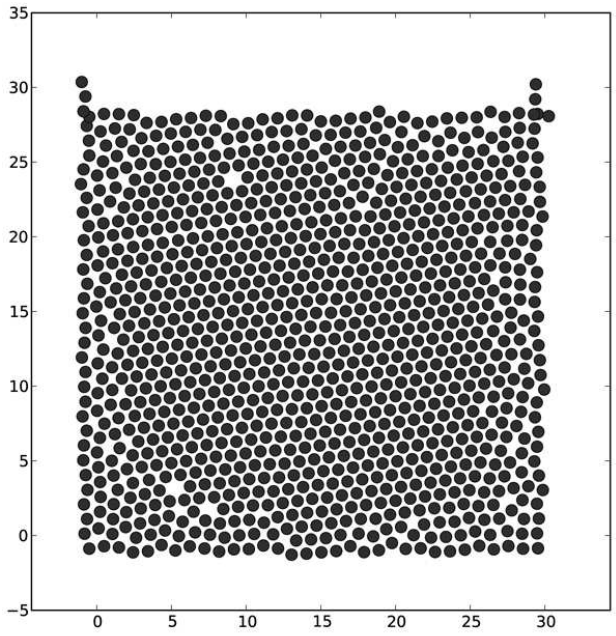

Figure 7: Arrangement of 900 elastic disks after the isotropic compression stage and some anisotropic compression cycles. The sample was initially ordered according to a square lattice, but the boundaries were irregular.

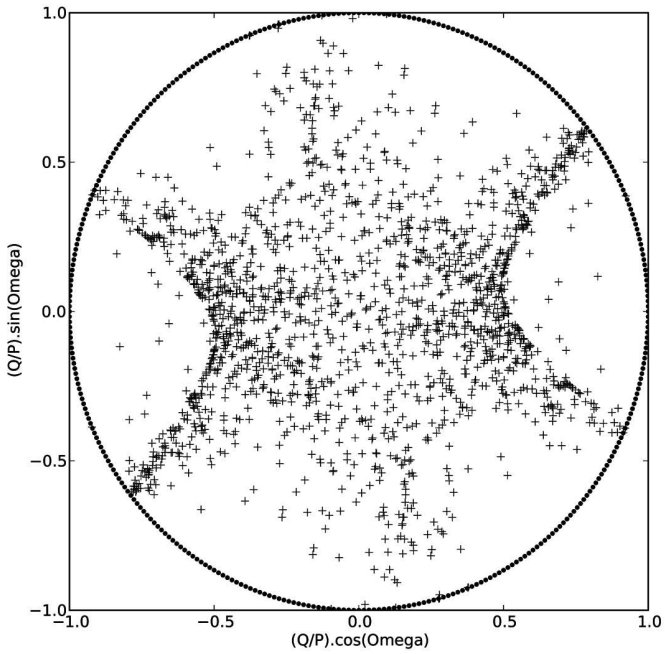

Figure 8: Distribution of points in the comparison plane of the simulation of isotropic compression of 900 disks after the isotropic compression stage and 4 anisotropic compression cycles. The number of particles is far from the thermodynamic limit conditions and most of the points are located within the respective allowed region of the corresponding *six-force* configuration associated to the main crystalline domain (Fig. 7).

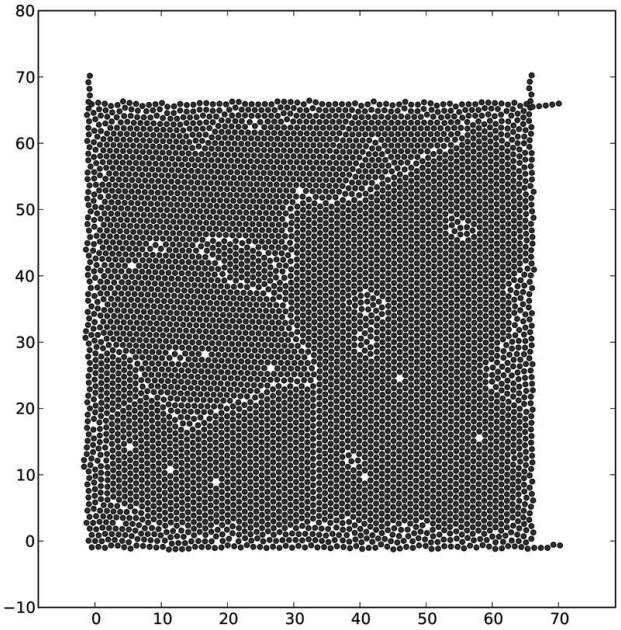

Figure 9: Arrangement of $4,900$ elastic disks after the isotropic compression stage. The sample was initially ordered according to a square lattice, but the boundaries were irregular. In this case, two main crystalline domains (grains) are found in the arrangement.

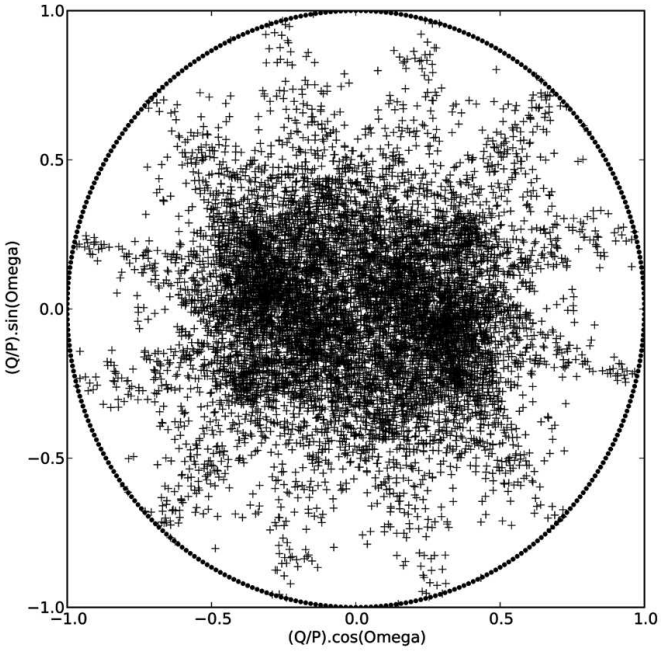

Figure 10: Distribution of points in the comparison plane of the $4,900$-disk compression simulation. It is still clear that the respective allowed regions of the two grains affect the statistical distribution of the points: two overlapping six-pointed stars can be discerned.